Slides, notes, and exercises at:
https://github.com/cheshyre/nptls-hf

Nuclear structure from the Hartree-Fock mean field

Nuclear Physics Turtle Lecture Series 2025:
Ab initio Hartree-Fock calculations of nuclei

Lecture 5

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NUCLEI
Nuclear Computational Low-Energy Initiative

Recap

- We can solve Hartree-Fock for some V_{NN}
- Inclusion of V_{3N} is challenging, but important

Main messages

- Three-nucleon forces are challenging to handle
- Can be efficiently approximated as **effective two-body interactions**
- **Three-body forces for cost of two-body forces,**
  makes large scale calculations possible
- Impact of 3N forces is essential
  - Repulsive contribution to binding energy
  - Impacts the location of drip lines
- **HF expectation values for other operators is easy**

HF with 3N forces on whiteboard

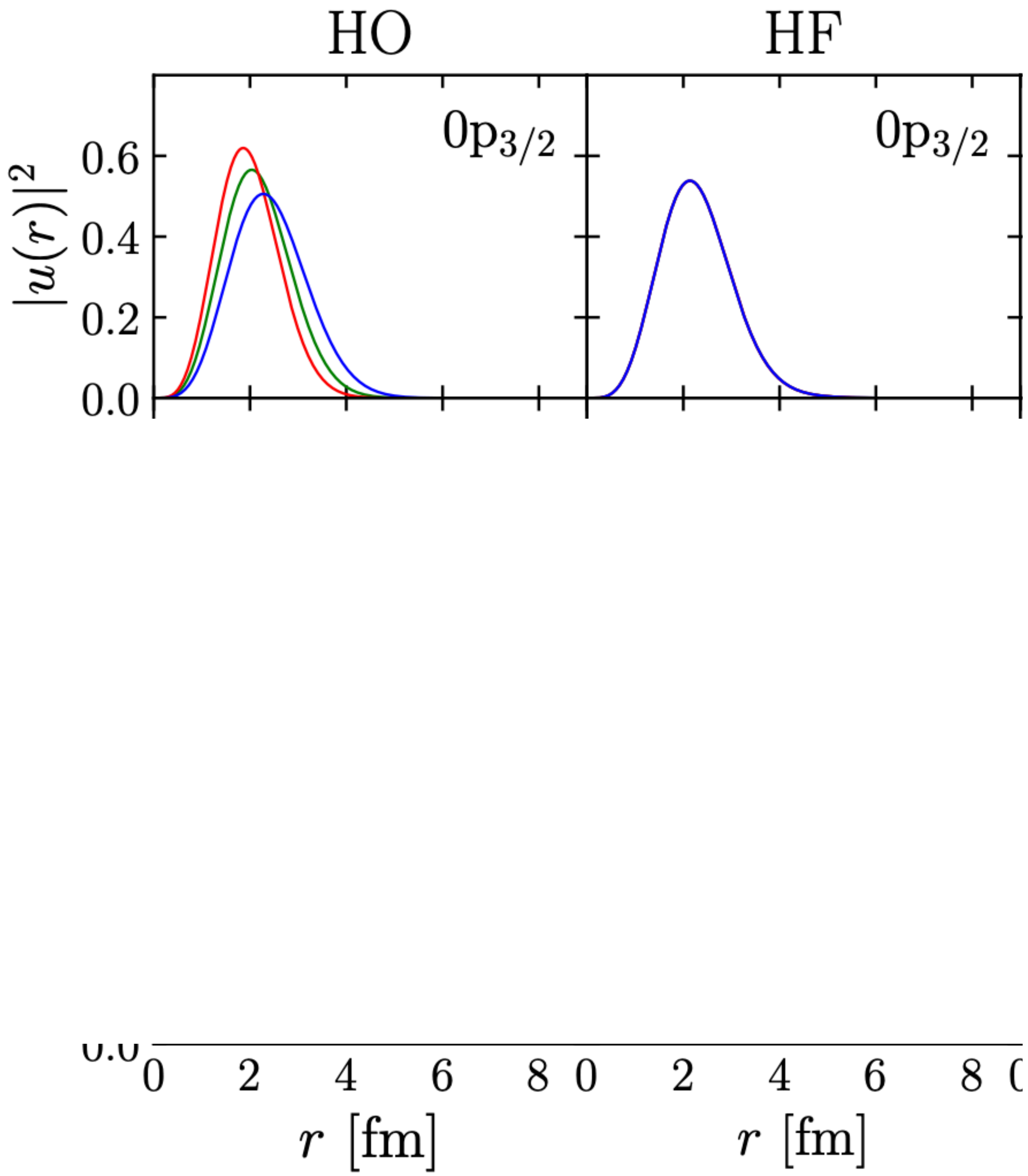
Orbital optimization

^{16}O

- Consider wave function $\langle \vec{r} \,|\, p \rangle = \phi_p(\vec{r})$
- Radial part $u_{nl}(r)/r$
- Angular part $Y_{lm}(\hat{r})$
- For occupied states, $u(r)$ becomes **independent** of $\hbar\omega$
- Unoccupied states are not optimized

different colors are different $\hbar\omega$

occupied



Tichai et al., PRC **99**, (2019)

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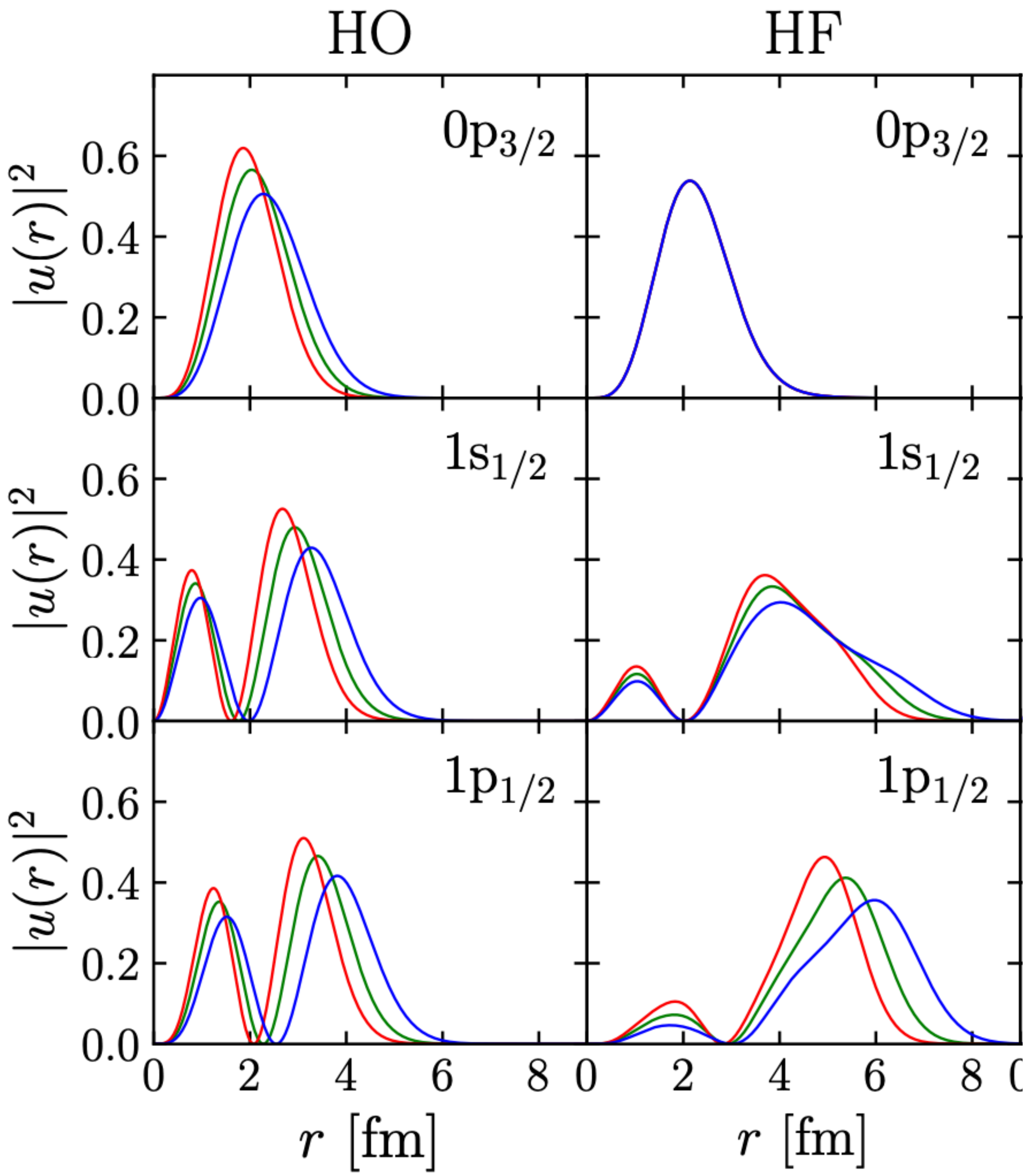

Tichai et al., PRC **99**, (2019)

Oxygen drip line and three-body forces

- Most of the time, **binding energy increases** as you add nucleons
- For very proton-rich or neutron-rich systems, binding energy begins to decrease again
  - System is **unbound** with respect to proton or neutron emission → drip line
- Calculations with only V_{NN}: oxygen isotopes more bound with more neutrons even beyond $^{24}\mathrm{O}$
- Calculations with V_{NN}, V_{3N}: neutron drip line at $^{24}\mathrm{O}$

$e_{\max} = 4$, **HF**

System	NN-only	NN + 3N
O-16	-150.81	-88.14
O-24	-217.35	-109.36
O-28	-232.73	-105.75

Our results!

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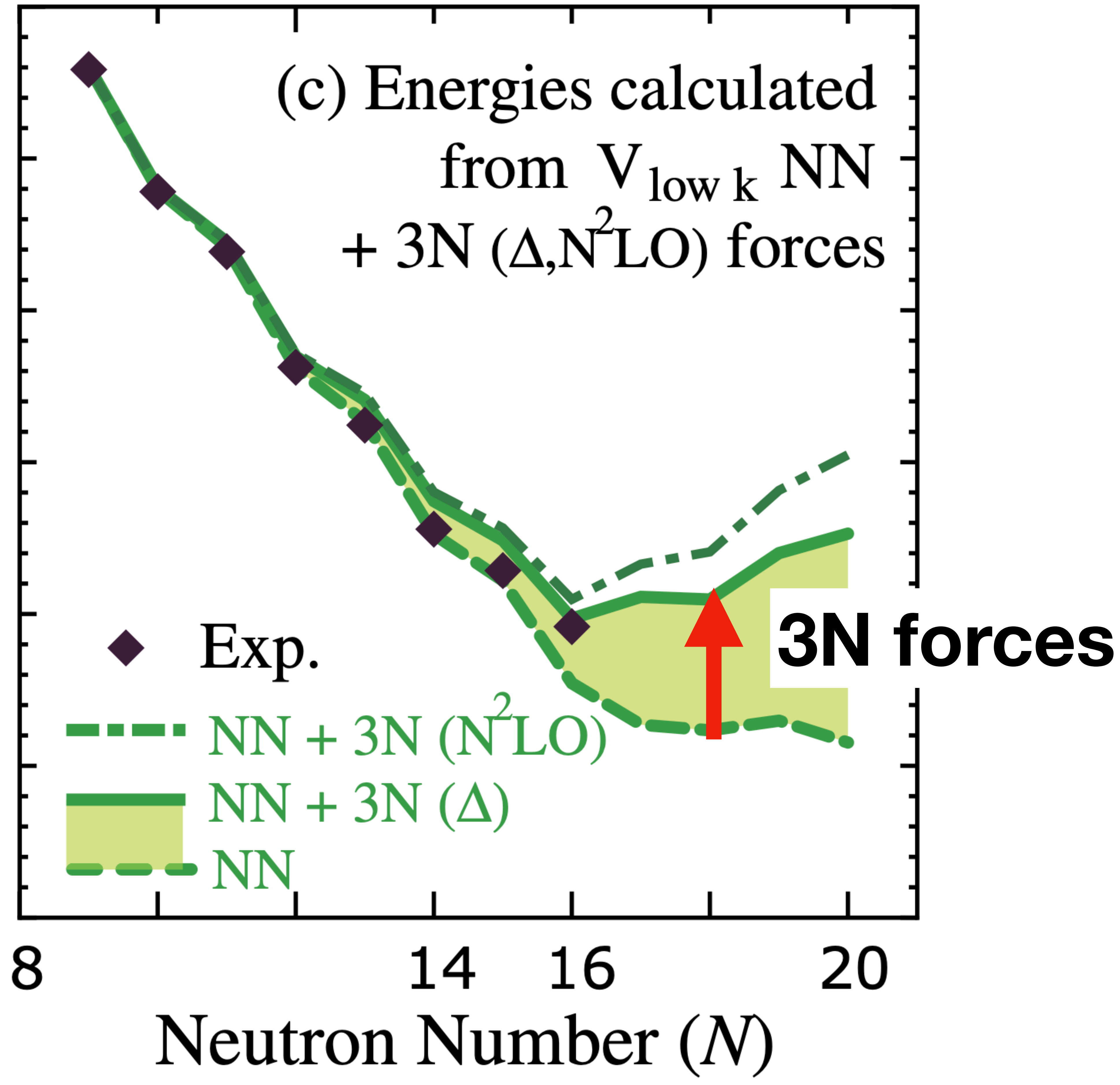
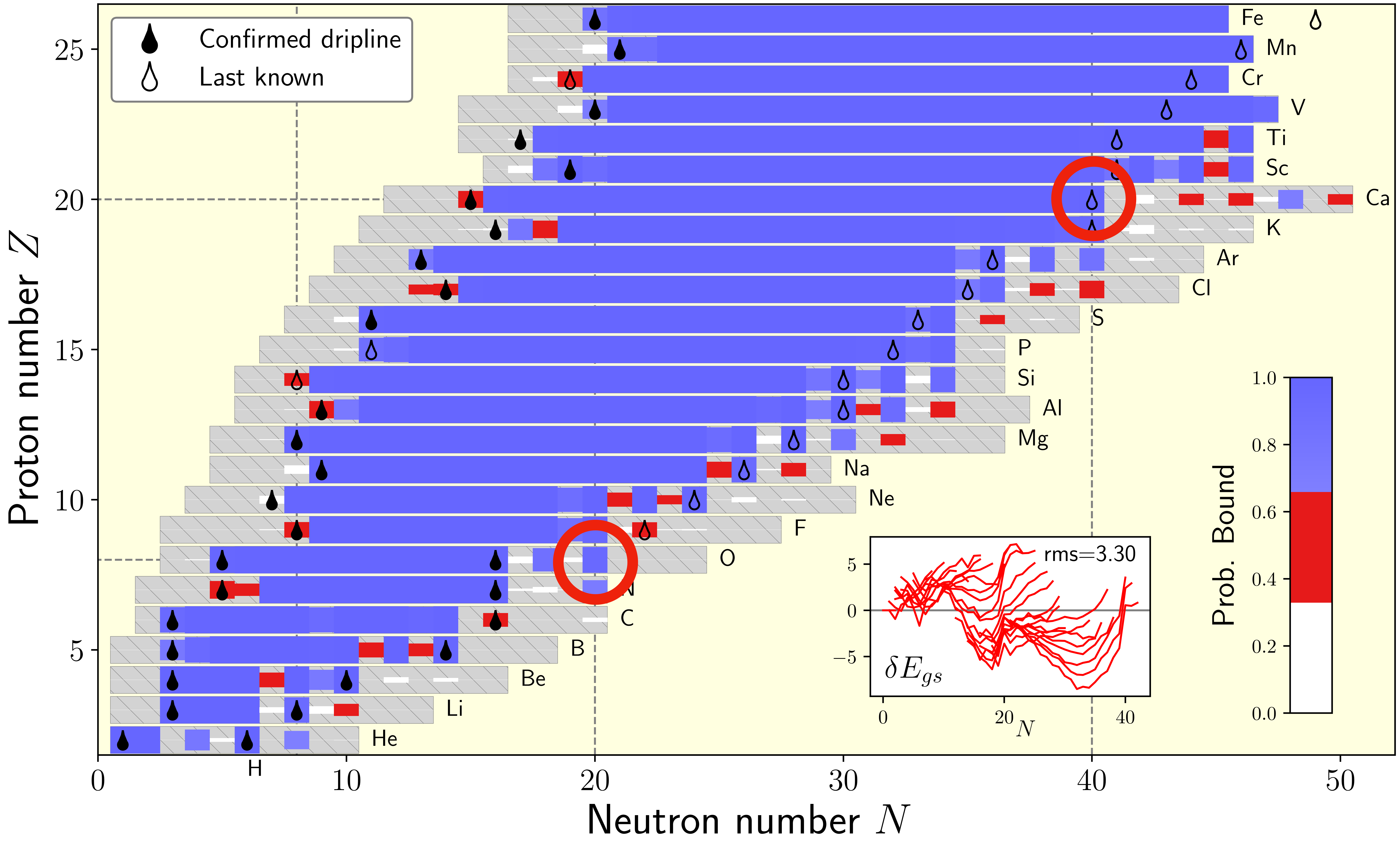


Otsuka et al., PRL **105**, (2010)

Global drip line predictions

- **Careful!**
- Not always so simple
- Some calculations still predict ^{28}O is bound
- Blue: likely bound
- Red: 50/50
- White: likely unbound



Stroberg et al., PRL **126** (2021)

Summary

- Can easily evaluate other operators at HF level
- Approximate 3-body forces as **effective 2-body forces**
- $$V_{pqrs}^{(3\mathrm{B,eff.})} = \sum_{tu} \rho_{tu} V_{pqtrsu}^{(3\mathrm{B})}$$
  - Modified prefactors, but treatment same as 2-body forces
- **Significant impact** in nuclear structure calculations
- But "**less important"** than 2-body forces?

What about bigger calculations?

- More clever treatment of symmetries of nuclear forces allows large e_{max}
  - Most important: **Rotational invariance**
  - Two-body matrix elements $\langle (pq)JM_J | V_{NN} | (rs)JM_J \rangle$ are diagonal in J, M_J and independent of M_J
  - Reduces storage cost by 100 to 1000
- Open-source codes available

Miyagi, EPJA **59**, 150 (2023)

  - NuHamil: https://github.com/Takayuki-Miyagi/NuHamil-public
  - imsrg++: https://github.com/ragnarstroberg/imsrg

NPTLS repository will be updated to allow you to reach $e_{\mathrm{max}} = 8$!